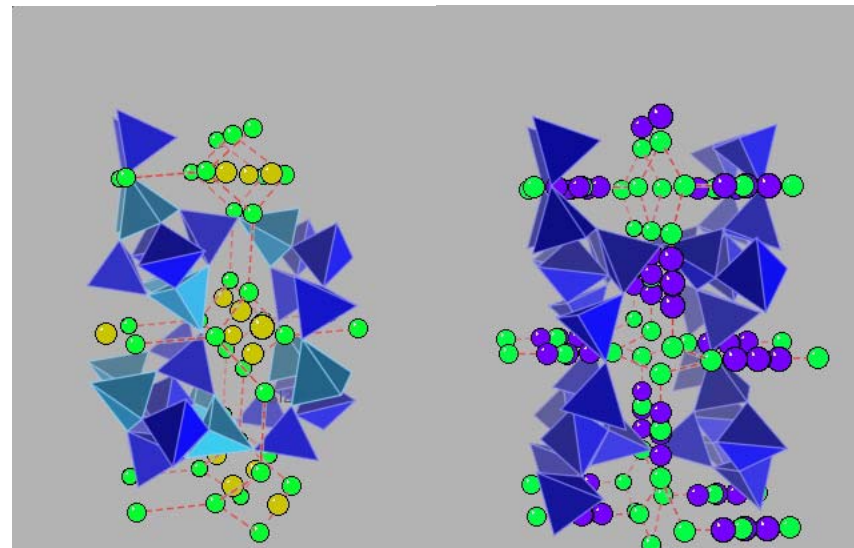


# Zeolites Expanding Under Pressure

John B. Parise, State University of New York, DMR-0095633

Microporous materials (“zeolites”) are important in processes such as ion exchange, gas separation, waste clean-up, detergent building and catalysis. Understanding the structure of this class of materials under a variety of environmental conditions is important to understanding their functionality. Studies at high pressure are now revealing a rich structural chemistry. In collaboration with co-workers at Brookhaven National Lab. and Birmingham, UK, we have discovered materials which expand under pressure. Some of these materials (GaSi-natrolite or NAT) are retained in the expanded state at room conditions where they display interesting ion exchange properties. We are evaluating the potential for ion capture when the expanded framework reverts to the “normal” (unexpanded) state.

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Views of the channel contents of Na-AlSi-NAT ( $\text{Na}_8\text{Al}_8\text{Si}_{12}\text{O}_{40} \cdot 8\text{H}_2\text{O}$ , left) and K-GaSi-NAT after pressure-induced hydration at 0.40 GPa and 1.9 GPa, respectively. Green circles represent water molecules which interact quite differently in the K (purple) and Na (yellow) variants. Hydrogen-bonding between water molecules is emphasized with dotted lines. Cation migration and differences in the water structure may be responsible for stabilizing the high water content form in the case of the GaSi framework; the AlSi reverts upon release of pressure.

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## Education:

Three undergraduates (Debbie Wang, Jonathan Rogers and Donique Jones), two graduate students (Aaron Celestian and Hyunsoo Park), and two postdocs (Yongjae Lee, now at BNL and Ivor Bull) contributed to this work. Undergraduates Donique Jones and Debbie Wang are biochemistry majors at Stony Brook while Rogers was an REU student in the summer of 2003 from Louisiana Technical University. All three under-graduate students are entering their senior year. Lee received his Ph.D. in 2001, and then worked as a postdoc in the group, where he started the high pressure (HP) work before transitioning to Brookhaven; in 2002 he received the van Valkenberg prize at the HP Gordon Conference and the Sinhu Award at the Pittsburg Diffraction Conference for the work described on the previous page

## Outreach:

With graduate student Celestian (top) and post doc Bull, the PI demonstrated the principles of ion exchange and real-time powder diffraction to Sayville high School students.

